

High Temperature Superconductivity from Strong Correlation

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Abstract

It is important to understand the mechanism of high-temperature superconductivity. It is obvious that the interaction with large energy scale is responsible for high critical temperature T_c . The Coulomb interaction is one of candidates that bring about high-temperature superconductivity because its characteristic energy is of the order of eV. There have been many works for the Hubbard model including three-band d-p model with the on-site Coulomb repulsion to investigate a possibility of high-temperature superconductivity. It is, of course, not trivial whether the on-site Coulomb interaction leads to a pairing interaction between two electrons. We argue that high-temperature superconductivity is possible in the strongly correlated region by using the variational Monte Carlo method for the two-dimensional t-U-J-V model. The exchange interaction J and the nearest-neighbour attractive interaction V cooperate with U and will act to enhance the critical temperature.

Keywords: high-temperature superconductor; strong correlation; Hubbard model; d-p model; t-U-J-V model; variational Monte Carlo method

1. Introduction

A basic question in the study of superconductivity is on an upper limit of the critical temperature T_c . It has been suggested that the maximum of T_c is in the range from 30K to 40K when the superconducting transition is based on the electron-phonon interaction [1, 2]. The prime reason of low T_c for the electron-phonon mechanism is that the Debye frequency ω_D is of the order of 100K and T_c is reduced by more than one digit than ω_D . In general, the electron-phonon coupling constant λ is small. Thus there is an upper limit for T_c within the electron-phonon mechanism. The interaction of large energy scale will be responsible for high temperature superconductivity. The electronic origin mechanisms of superconductivity are worth studying in the search of high temperature superconductors. The electronic interaction comes from the Coulomb interaction between electrons. From this point of view, it is important to consider the intra-atomic Coulomb interactions that are of the order of eV. Then a question arises as to whether the superconductivity is indeed induced by the Coulomb interaction. This subject has been studied intensively by using electronic models with the on-site Coulomb interaction U including the two-dimensional (2D) Hubbard model [3-26], the d-p model [27-33] and also the ladder Hubbard model [34-38].

It remains matter of controversial as to whether the 2D Hubbard model accounts for high-temperature superconductivity. Most of the results of quantum Monte Carlo methods have failed to show the existence of superconductivity [13,14,18], and some results, however, still keep open the possibility of superconductivity [15, 24]. We must note that quantum Monte Carlo methods are methods being applicable only in the weakly correlated region where U/t is not large and is at most from 4 to

5. The existence of superconductivity in strongly correlated regions should be considered further. This may account for properties of high-temperature cuprate superconductors.

2. Superconductivity in Strongly Correlated Region

Superconductivity in the strongly correlated region is described by using the 2D Hubbard model. The Hamiltonian is given by

$$H = \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

$\{t_{ij}\}$ are transfer integrals and U is the on-site Coulomb energy. The transfer integral t_{ij} is non-zero $t_{ij} = t$ for nearest-neighbor pair $\langle ij \rangle$ and $t_{ij} = t$ for next-nearest neighbor pair $\langle ij \rangle$; otherwise t_{ij} vanishes. We denote the number of sites as N and the number of electrons as N_e .

The ground state of the Hubbard model is divided into two regions, that is, a weak correlation region and a strong correlation region. When the Coulomb interaction U is as large as or greater than the bandwidth $8t$, the ground state should be regarded as the strongly correlated one [39, 40]. We use the Gutzwiller ansatz and evaluate the superconducting condensation energy E_{cond} for d-wave pairing. The wave function is

$$\psi = P_{N_e} P_G \psi_{BCS}, \quad (2)$$

where P_G is the Gutzwiller operator $P_G = \prod_j (1 - (1-g)n_{j\uparrow}n_{j\downarrow})$ with the parameter g in the range of $0 \leq g \leq 1$. The gap function Δ in the BCS function ψ_{BCS} is regarded as a variational parameter. P_{N_e} is a projection operator that extracts only the state with a fixed total electron number N_e . The condensation

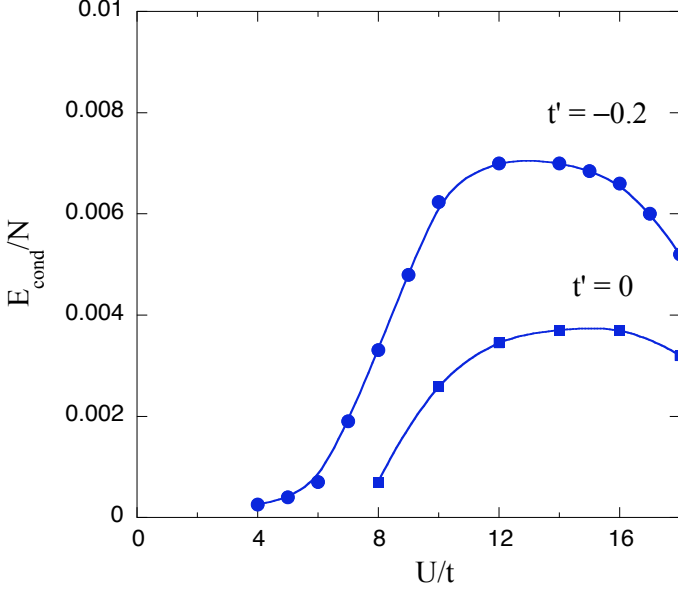


Figure 1: The superconducting condensation energy per site as a function of U in units of t for $t = 0$ and $t = 0.2$ on 10×10 lattice. The number of electrons is $N_e = 88$ for $t = 0$ and $N_e = 84$ for $t = 0.2$.

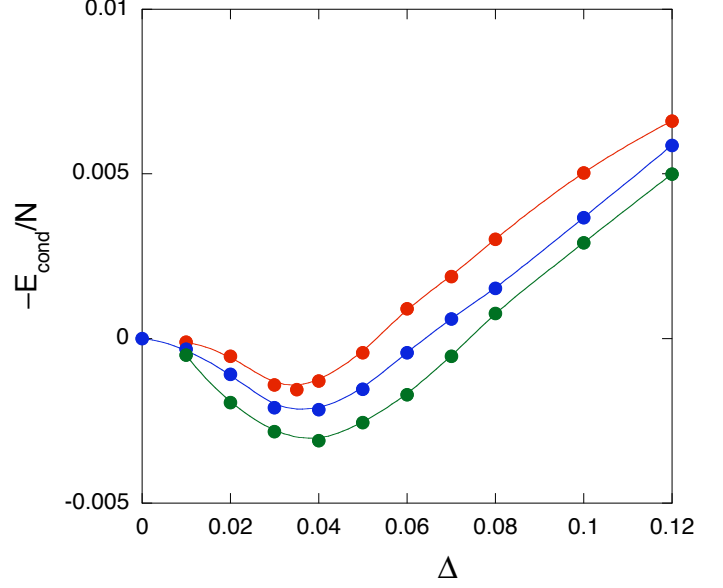


Figure 2: The superconducting condensation energy per site as a function of Δ in units of t . From the top, we set $J = 0, 0.1$ and 0.3 for parameters $U = 12$ and $t = 0.2$. The number of electron is $iN_e = 84$ on 10×10 lattice.

energy is defined as $E_{cond} = E(\Delta = 0) - E(\Delta = \Delta_{opt})$ for the optimized gap function Δ_{opt} .

We show E_{cond} as a function of U in Fig.1. E_{cond} increases rapidly near $U \sim 8t$ as going into the strongly correlated region. E_{cond} is very small in the weakly correlated region for $U < 8t$ and almost vanishes for $t = 0$. For such small value of E_{cond} , it is certainly hard to obtain a signal of superconductivity by means of numerical methods such as the quantum Monte Carlo method. It follows from Fig.1 that high temperature superconductivity is possible only in the strongly correlated region. In particular, $U/t \sim 10 - 14$ is favorable for superconductivity. Similar results have been reported for $t/t = 0.1, 0.25$ and 0.4 in Ref. [26].

3. Enhancement of Superconductivity with Weak Attractive Interactions

Let us examine when the critical temperature T_c is enhanced in correlated-electron systems. A layered crystal structure is obviously an important factor. The increase of the density of states in a layered crystal is certainly important and an inter-layer interaction plays a significant role in finding new superconductors [41-45]. Apart from this, if there is an interaction that promotes superconductivity cooperating with the Coulomb interaction, T_c will be increased. The d -wave pairing state in the Hubbard model will be more stabilized by weak nearest-neighbor attractive interactions. We consider the exchange interaction J and attractive interaction V given as

$$H = \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + J \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) + V \sum_{\langle ij \rangle} n_i n_j. \quad (3)$$

This is so called the t - U - J - V model. In high-temperature cuprates, the exchange coupling J arises as a super-exchange interaction between d electrons in copper atoms, which is mediated by oxygen atoms. The last term with negative V is expected to arise from the electron-phonon interaction [46]. In the variational Monte Carlo calculations, both J and V (< 0) act as an attractive interaction for nearest-neighbour pairs of electrons. The Gutzwiller ansatz is also adopted here. We use the electron-hole transformation to fix the electron number in ψ_{BCS} instead of using P_{N_e} [47]. We show the results in Figs.2 and 3. In Fig.2 we compare E_{cond} for $J/t = 0, 0.1$ and 0.2 where $U/t = 12$ and $t/t = 0.2$. Basically the exchange coupling J works effectively in a similar way to U to form the d -wave pairing. We obtain a similar result for the interaction V , where the lowering of the energy E_{cond} by V is smaller than that by J . It should be noted, however, that J alone can not stabilize the d -wave pairing, which means that if U is small, the d -wave superconducting state is not realized even for $J > 0$. This is shown in Fig.3 where E_{cond} is shown as a function Δ with $J = 0.1$ and $t = 0$ for $U/t = 8$ and 12 . E_{cond} is very small for $U/t = 8$ and vanishes for small U . This indicates that the strong on-site correlation is needed so that the exchange coupling J induces superconductivity.

4. Summary

We have investigated the two-dimensional t - U - J - V Hubbard model. The condensation energy becomes large in the strongly correlated region, suggesting a possibility of high-temperature superconductivity. We mention here that there is a report that suggests a high-temperature superconductivity in the moderate- U region by means of the dynamical mean field theory [25]. We

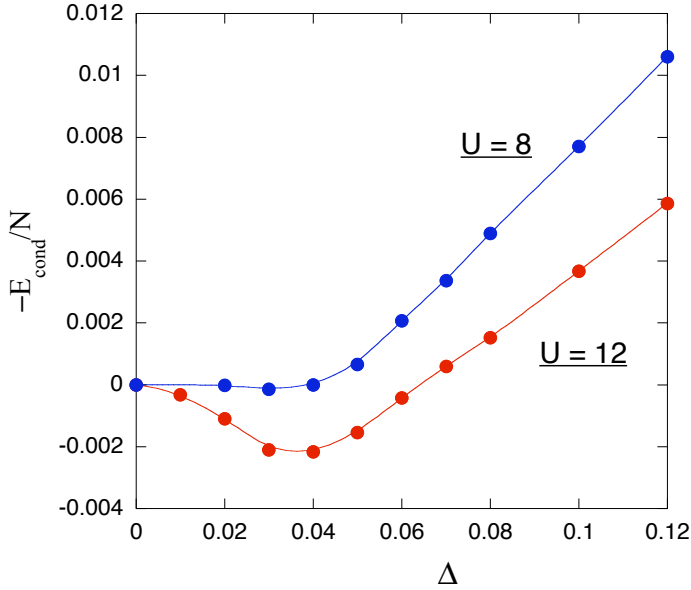


Figure 3: The superconducting condensation energy per site as a function of Δ in units of t . The condensation energy as a function of Δ in units of t for $J = 0.1$ and $t = 0$ where $U = 8$ and $U = 12$.

must further clarify a consistency with the results obtained by the quantum Monte Carlo method.

The exchange interaction J and the nearest-neighbor attractive interaction V cooperate with the Coulomb interaction U to enhance superconductivity. It is important that the exchange coupling J alone cannot promote superconductivity if U is small in the weakly correlated region. We expect that the strong U and weak J and V may realize high critical temperature

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References

- [1] W. L. McMillan, Phys. Rev. 167 (1968) 331.
- [2] P. B. Allen, R. C. Dynes, Phys. Rev. B12 (1975) 905.
- [3] J. E. Hirsch, Phys. Rev. B31 (1985) 4403.
- [4] H. Yokoyama, H. Shiba, J. Phys. Soc. Jpn. 57 (1988) 2482.
- [5] S. R. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh, J. E. Gubernatis, R. T. Scalettar, Phys. Rev. B40 (1989) 506.
- [6] J. E. Hirsch, D. Loh, D. J. Scalapino, S. Tang, Phys. Rev. B39 (1989) 243.
- [7] R. T. Scalettar, D. J. Scalapino, R. L. Sugar, S. R. White, Phys. Rev. B39 (1989) 243.
- [8] A. Moreo, Phys. Rev. B45 (1992) 5059.
- [9] T. Yanagisawa, Y. Shimoi, Int. J. Mod. Phys. B10 (1996) 3383.

- [10] T. Nakanishi, K. Yamaji and T. Yanagisawa, J. Phys. Soc. Jpn. 66 (1997) 294.
- [11] K. Yamaji, T. Yanagisawa, T. Nakanishi and S. Koike, Physica C304 (1998) 225.
- [12] K. Yamaji, T. Yanagisawa and S. Koike, Physica B284 (2000) 415.
- [13] S. Zhang, J. Carlson and J. E. Gubernatis, Phys. Rev. B55 (1997) 7464.
- [14] S. Zhang, J. Carlson and J. E. Gubernatis, Phys. Rev. Lett. 78 (1997) 4486.
- [15] K. Kuroki, H. Aoki, Phys. Rev. B56 (1997) R14287.
- [16] N. Bulut, Advances in Phys. 51 (2002) 1587.
- [17] M. Miyazaki, T. Yanagisawa, K. Yamaji, J. Phys. Soc. Jpn. 73 (2004) 1643.
- [18] T. Aimi, M. Imada, J. Phys. Soc. Jpn. 76 (2007) 113708.
- [19] M. Miyazaki, K. Yamaji, Y. Yanagisawa, R. Kadono, J. Phys. Soc. Jpn. 78 (2009) 043706.
- [20] K. Yamaji, T. Yanagisawa, M. Miyazaki, R. Kadono, J. Phys. Soc. Jpn. 80 (2011) 083702.
- [21] J. Kondo, J. Phys. Soc. Jpn. 70 (2001) 808.
- [22] R. Hlubina, Phys. Rev. B59 (1999) 9600.
- [23] T. Yanagisawa, New J. Phys. 10 (2008) 023014.
- [24] T. Yanagisawa, New J. Phys. 15 (2013) 033012.
- [25] E. Gull, O. Parcdlet, A. J. Millis, Phys. Rev. Lett. 110 (2013) 216405.
- [26] H. Yokoyama, M. Ogata, Y. Tanaka, K. Kobayashi, H. tsuchiura, J. Phys. Soc. Jpn. 82 (2013) 014707.
- [27] V. J. Emery, Phys. Rev. Lett. 58 (1997) 2794.
- [28] C. Weber, A. Lauchi, F. Mila, T. Giamarchi, Phys. Rev. Lett. 102 (2009) 017005.
- [29] B. Lau, M. Berciu, G. A. Sawatzky, Phys. Rev. Lett. 106 (2011) 036401.
- [30] T. Yanagisawa, S. Koike, K. Yamaji, Phys. Rev. B64 (2001) 184509.
- [31] T. Yanagisawa, S. Koike, K. Yamaji, Phys. Rev. B67 (2003) 132408.
- [32] T. Yanagisawa, M. Miyazaki, K. Yamaji, J. Phys. Soc. Jpn. 78 (2009) 013706.
- [33] T. Yanagisawa, M. Miyazaki, K. Yamaji, J. Mod. Phys. 4 (2013) 33.
- [34] R. M. Noack, N. Bulut, D. J. Scalapino, M. G. Zacher, Phys. Rev. B56 (1997) 7162.
- [35] K. Kuroki, T. Kimura, H. Aoki, Phys. Rev. B54 (1996) R15641.
- [36] S. Koike, K. Yamaji, T. Yanagisawa, J. Phys. Soc. Jpn. 68 (1999) 1657.
- [37] K. Yamaji, Y. Shimoi, T. Yanagisawa, Physica C235-240 (1994) 2221.
- [38] T. Yanagisawa, Y. Shimoi, K. Yamaji, Phys. Rev. B52 (1995) R3860.
- [39] H. Yokoyama, M. Ogata, Y. Tanaka, J. Phys. Soc. Jpn. 95 (2006) 114906.
- [40] T. Yanagisawa, M. Miyazaki, Europhys. Lett. 107 (2014) 27004.
- [41] Y. Maeno, H. Hashimoto, K. Yoshida, S. Nishizaki, T. Fujita, J. G. Bednorz, F. Lichtenberg, Nature 372 (1994) 532.
- [42] A. F. Hebard, M. J. Rosseinsky, R.C. Haddon, D. W. Murphy, S. H. Glarum, T. T. Palstra, A. P. Ramirez, A.R. Kortan, Nature 350 (1991) 600.
- [43] J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitani, J. Akimitsu, Nature 410 (2001) 63.
- [44] S. Koikegami and T. Yanagisawa, J. Phys. Soc. Jpn. 75 (2006) 034715; S. Koikegami and T. Yanagisawa, J. Phys. Soc. Jpn. 70 (2001) 3499; ibid. 71 (2002) 671 (E).
- [45] S. Koikegami and T. Yanagisawa, Phys. Rev. B67 (2003) 134517.
- [46] T. M. Hardy, J. P. Hague, J. H. Samson, A. S. Alexandrov, Phys. Rev. B79 (2009) 212501.
- [47] T. Yanagisawa, S. Koike, K. Yamaji, J. Phys. Soc. Jpn. 67 (1998) 3867; T. Yanagisawa, S. Koike, K. Yamaji, J. Phys. Soc. Jpn. 68 (1999) 3608.